



**RICHARD P.
FEYNMAN**
CENTER FOR INNOVATION
at Los Alamos National Laboratory

Advance a Ligand and Homogenous Catalysis Platform

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Request for Information

Los Alamos National Security, LLC (LANS) is the manager and operator of Los Alamos National Laboratory (Los Alamos) for the U.S. Department of Energy National Nuclear Security Administration under contract DE-AC52-06NA25396. Los Alamos is a mission-centric Federally Funded Research and Development Center focused on solving critical national security challenges through science and engineering for both government and private customers. LANS is opening this formal Request for Information (RFI) to gauge interest in engaging as an industry partner with LANS for collaboration in advancing the ligand and catalyst platform described below. Please see last section for details on submitting a Letter of Interest.

A Versatile Ligand and Metal Complex Toolbox

The vast majority of ligands used in industrial homogeneous catalysis are based on P and/or N donor atoms, with an enormous number of such ligands having been designed and synthesized over the past five decades. Among these are polydentate chelating ligands bearing N–H functionalities that are currently accepted to play a crucial role in so-called “metal-ligand bifunctional catalysis”. A representative example is the commercially available PNP ligand family, of general formula $R_2P(CH_2)_2NH(CH_2)_2PR_2$, members of which have been known since the 1970s. These ligands, as well as many others based on phosphorus, are usually difficult to synthesize on a multigram scale, are costly and are typically susceptible to oxidation at the phosphorus. Success in catalysis science relies on the development of new and novel ligands. Los Alamos researchers have recently developed ENENES, NN and SNNS – three new families of phosphorous-free ligands. Advantages of these ligands include:

- Ease of synthesis from commercially available, inexpensive starting materials at the multi-gram scale;
- Scalability of synthesis (multi-gram quantities are easily accessible in one loading);
- Ability to readily change the number of carbon atoms in ligand backbone (unlike PNP systems);
- Tunability of electronics and sterics (e.g. facile addition of various substituents at N and S centers);
- Chirality;
- Air stability;
- Demonstrated good activity in carbonyl group catalytic hydrogenations and transfer hydrogenations;
- Potential activity in numerous other catalytic reactions (see below).

Ligands and Complexes for Homogenous Catalysis

Los Alamos scientists have prepared new ligands from inexpensive starting materials, and new metal complexes with these ligands, investigating their activity and selectivity towards the hydrogenation of carbonyl containing compounds (e.g. simple and functionalized ketones, esters). Several structurally unprecedented catalysts have been synthesized, and the hydrogenation of esters and ketones has been demonstrated with high activities and selectivities. This technology represents a new alternative to PNP-based systems that may have the potential for efficacy in numerous catalytic reactions, including but not limited to:

- Asymmetric catalysis
- Hydrogenating unsaturated substrates, e.g.:
 - Alkenes
 - Alkynes
 - Carbonic & carboxylic acid derivatives
 - CO₂
 - Esters
 - Fluorinated esters
 - Heterocycles
 - Imines
 - Ketones
 - Formates
 - Cyclic carbonates
- Catalytic hydrolysis or dehydrogenation of ammonia or amine boranes
- Various acceptorless dehydrogenations
- Various dehydrations
- Polymerizing alkenes
- Transfer hydrogenation of ketones, organic formates and cyclic carbonates
- Domino-synthesis of indoles
- Stereospecific polymerization of 1,3-butadiene
- Ethylene tetra- and trimerisation
- Other types of catalysis

Potential Areas for Partnership

- Design of scale-up synthetic chemistry to produce catalysts and/or ligands for large-scale distribution.
- Test & evaluation of catalysts and/or ligands for applications in the pharmaceutical, petrochemical & renewable energy, agrochemical, consumer products, fine chemicals, polymers, flavors & fragrances, advanced materials, bioderived materials, biologics, or other applications.
- Vending of the catalysts and/or ligands to third parties.

Please note this list is non-exhaustive. LANS welcomes Letters of Interest from any suitable party, and is not necessarily limited to one partner per area of interest.

LANS Intellectual Property

Polydentate ligands and their complexes for molecular catalysis (LANS Ref. No. S 133,200; PCT App. No. PCT/US2015/034793) Catalytic hydrogenation using complexes of base metals with tridentate ligands (LANS Ref. No. S 129,408; U.S. Pat. App. No. 13/587,717)

Please note that the U.S. Government retains a worldwide, royalty-free, non-exclusive right to practice any LANS-owned patents and/or copyrighted software. Accordingly, any entity will have open access to LANS patents and copyrights in performance of a Government contract.

Submitting a Letter of Interest

This RFI is made without prejudice to any form of collaborative arrangement, alliance, or number of entities. Ability and willingness to ensure compliance with U.S. Export Control law is a requirement. Please submit a written response on how your organization envisions utilizing this technology in partnership with Los Alamos. This may include a business or product plan, a business model, information regarding your company, or any other type of relevant information. Please properly mark any information that is considered proprietary or business-sensitive. LANS will supply a Nondisclosure Agreement to any U.S. company or person requiring it.

Those companies interested in pursuing this opportunity should direct a Letter of Interest, as well as any comments or questions, to catalysis@lanl.gov before 11:59 MST on April 29, 2016.

Download this [Request for Interest \(pdf\)](#).

RICHARD P. FEYNMAN CENTER FOR INNOVATION

www.lanl.gov/feynmancenter | (505) 667-9090 | feynmancenter@lanl.gov